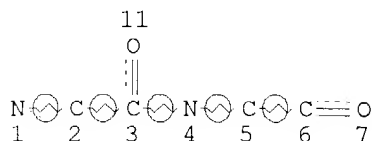


=&gt; d que 122

L14 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

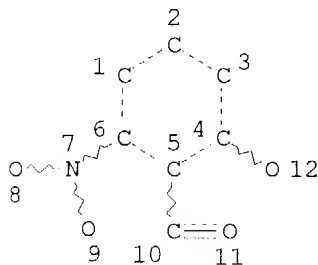
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

L16 90710 SEA FILE=REGISTRY SSS FUL L14

L18 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L20 393 SEA FILE=REGISTRY SSS FUL L18

L22 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L16 AND L20

=&gt; d 122 ibib abs hitstr 1-4

L22 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:501665 HCAPLUS

DOCUMENT NUMBER: 139:197756

TITLE: Difficult Macrocyclizations: New Strategies for  
 Synthesizing Highly Strained Cyclic Tetrapeptides  
 AUTHOR(S): Meutermans, Wim D. F.; Bourne, Gregory T.; Golding,  
 Simon W.; Horton, Douglas A.; Campitelli, Marc R.;  
 Craik, David; Scanlon, Martin; Smythe, Mark L.

CORPORATE SOURCE: Institute for Molecular Bioscience, University of  
 Queensland, St. Lucia, 4072, Australia

SOURCE: Organic Letters (2003), 5(15), 2711-2714  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 139:197756

AB To synthesize highly strained cyclic tetrapeptides, the authors developed a macrocyclization strategy that involves the inclusion of 2-hydroxy-6-nitrobenzyl (HnB) as an N-protective group at the N-terminus and in the "middle" of the sequence. The N-terminal auxiliary performs a ring closure/ring contraction role, and the backbone auxiliary promotes cis amide bonds to facilitate the otherwise difficult ring contraction. Following this route, the all-L cyclo[Tyr-Arg-Phe-Ala] was successfully prepared

IT 583051-34-7P 583051-36-9P

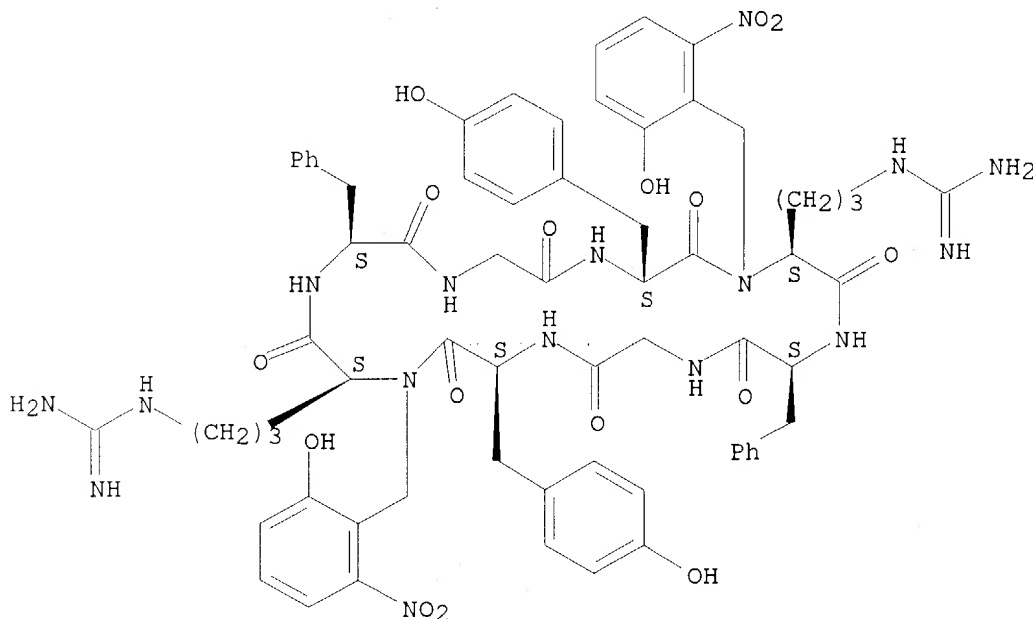
RL: BYP (Byproduct); PREP (Preparation)

(preparation of highly strained cyclic tetrapeptides via cyclizations of linear peptides containing N-protecting hydroxynitrobenzyl groups)

RN 583051-34-7 HCAPLUS

CN Cyclo[N2-[(2-hydroxy-6-nitrophenyl)methyl]-L-arginyl-L-phenylalanylglycyl-L-tyrosyl-N2-[(2-hydroxy-6-nitrophenyl)methyl]-L-arginyl-L-phenylalanylglycyl-L-tyrosyl] (9CI) (CA INDEX NAME)

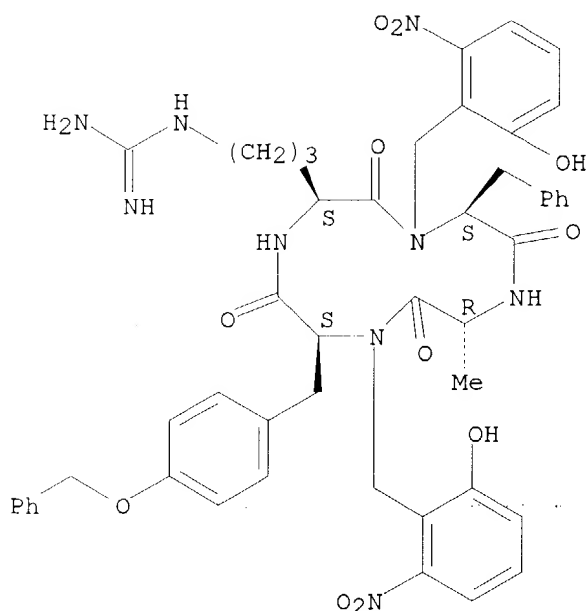
Absolute stereochemistry.



RN 583051-36-9 HCAPLUS

CN Cyclo[D-alanyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-O-(phenylmethyl)-L-tyrosyl-L-arginyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-phenylalanyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



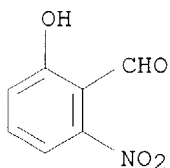
IT 16855-08-6, 2-Hydroxy-6-nitrobenzaldehyde

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of highly strained cyclic tetrapeptides via cyclizations of linear peptides containing N-protecting hydroxynitrobenzyl groups)

RN 16855-08-6 HCAPLUS

CN Benzaldehyde, 2-hydroxy-6-nitro- (9CI) (CA INDEX NAME)



IT 263276-96-6P 263277-01-6P 263277-08-3P

263277-33-4P 583051-15-4P 583051-37-0P

583051-38-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

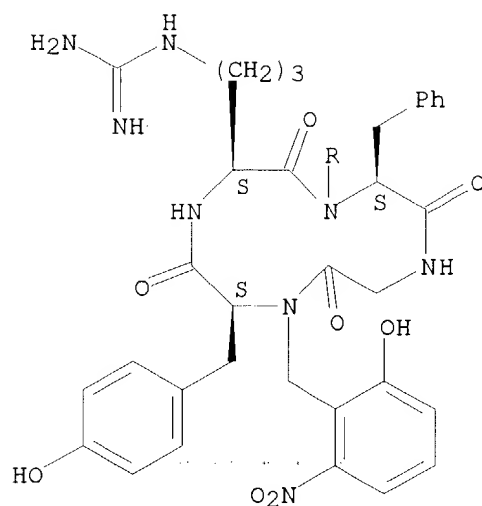
(preparation of highly strained cyclic tetrapeptides via cyclizations of linear peptides containing N-protecting hydroxynitrobenzyl groups)

RN 263276-96-6 HCAPLUS

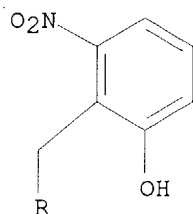
CN Cyclo[L-arginyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-phenylalanylglycyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-tyrosyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



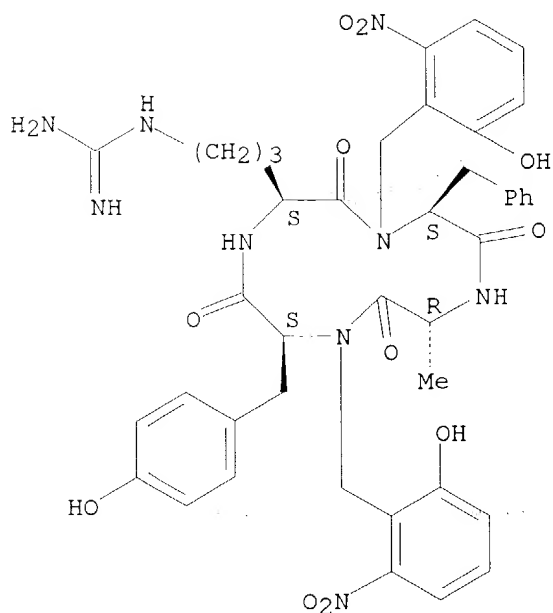
PAGE 2-A



RN 263277-01-6 HCAPLUS

CN Cyclo[D-alanyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-tyrosyl-L-arginyl-N-  
 [(2-hydroxy-6-nitrophenyl)methyl]-L-phenylalanyl] (9CI) (CA INDEX NAME)

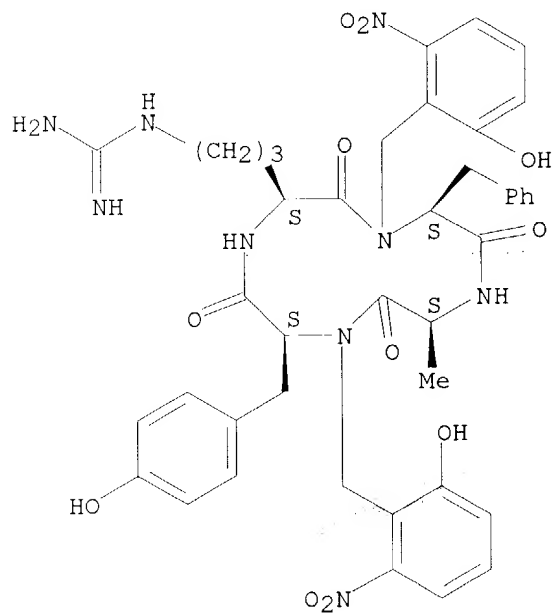
Absolute stereochemistry.



RN 263277-08-3 HCAPLUS

CN Cyclo[L-alanyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-tyrosyl-L-arginyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-phenylalanyl] (9CI) (CA INDEX NAME)

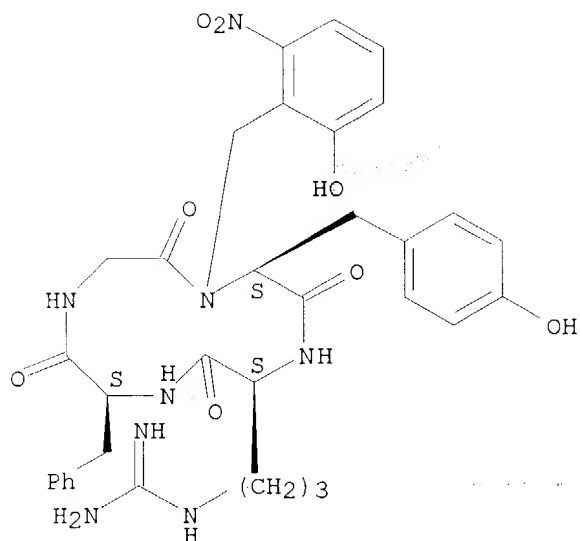
Absolute stereochemistry.



RN 263277-33-4 HCAPLUS

CN Cyclo[L-arginyl-L-phenylalanylglycyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-tyrosyl] (9CI) (CA INDEX NAME)

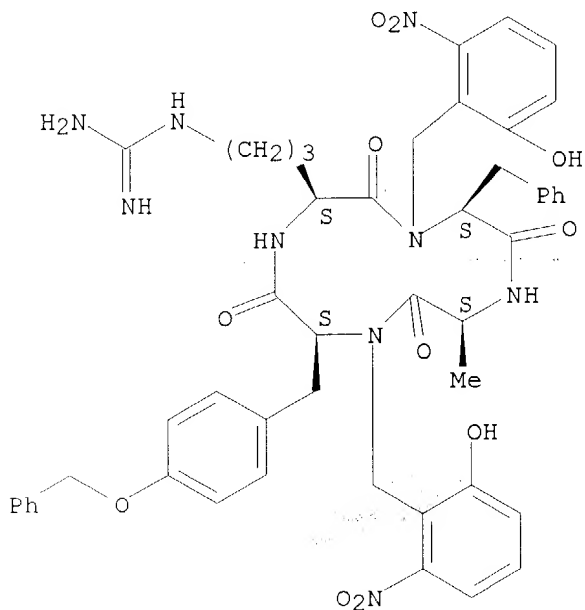
Absolute stereochemistry.



RN 583051-15-4 HCAPLUS

CN Cyclo[L-alanyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-O-(phenylmethyl)-L-tyrosyl-L-arginyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-phenylalanyl]  
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

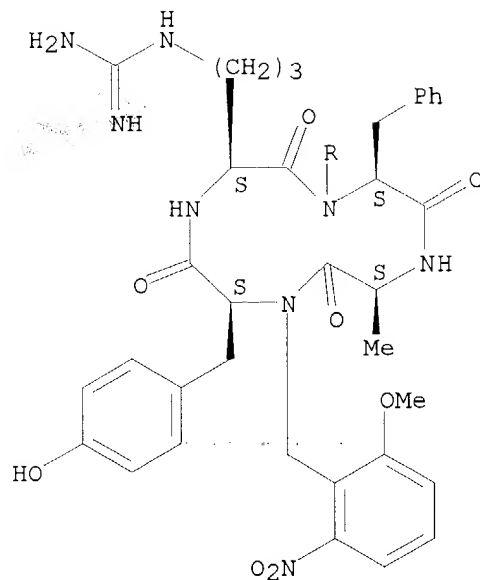


RN 583051-37-0 HCAPLUS

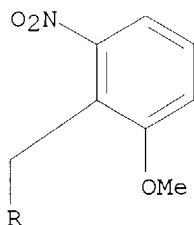
CN Cyclo[L-alanyl-N-[(2-methoxy-6-nitrophenyl)methyl]-L-tyrosyl-L-arginyl-N-[(2-methoxy-6-nitrophenyl)methyl]-L-phenylalanyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



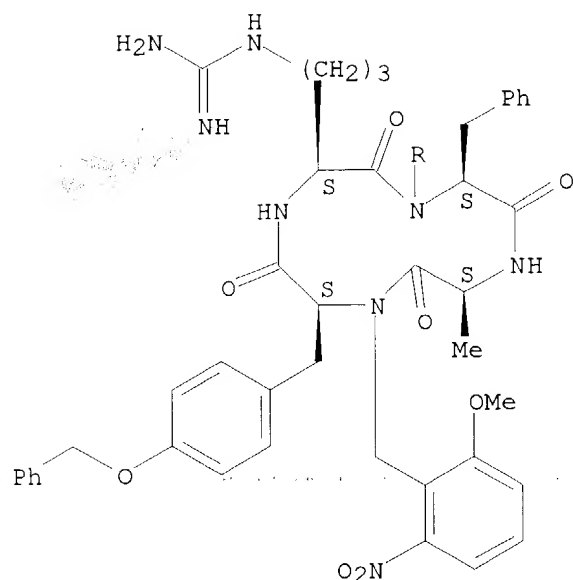
PAGE 2-A



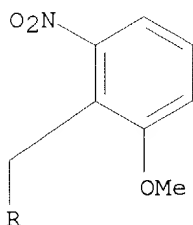
RN 583051-38-1 HCAPLUS  
 CN Cyclo[L-alanyl-N-[(2-methoxy-6-nitrophenyl)methyl]-O-(phenylmethyl)-L-tyrosyl-L-arginyl-N-[(2-methoxy-6-nitrophenyl)methyl]-L-phenylalanyl]  
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



IT 263144-23-6P 263277-02-7P 583051-18-7P  
583051-22-3P 583051-31-4P

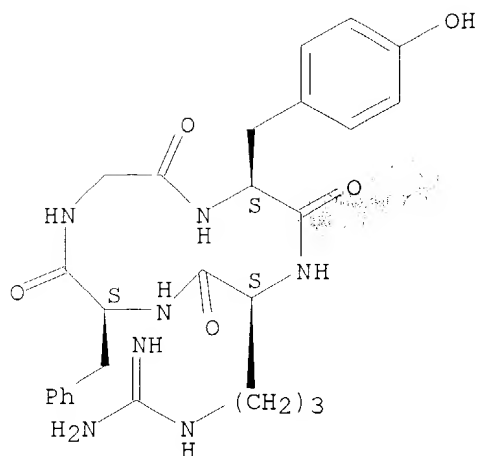
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of highly strained cyclic tetrapeptides via cyclizations of  
linear peptides containing N-protecting hydroxynitrobenzyl groups)

RN 263144-23-6 HCAPLUS

CN Cyclo(L-arginyl-L-phenylalanylglycyl-L-tyrosyl) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

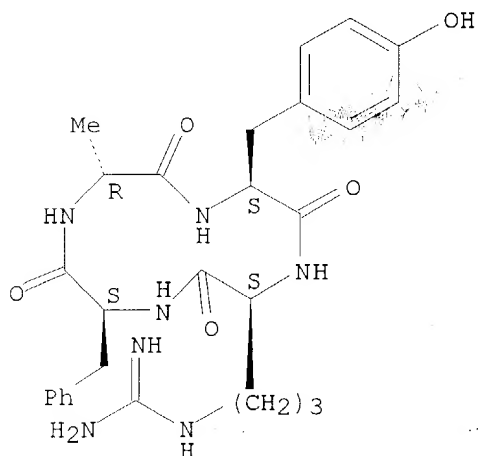




RN 263277-02-7 HCAPLUS

CN Cyclo(D-alanyl-L-tyrosyl-L-arginyl-L-phenylalanyl) (9CI) (CA INDEX NAME)

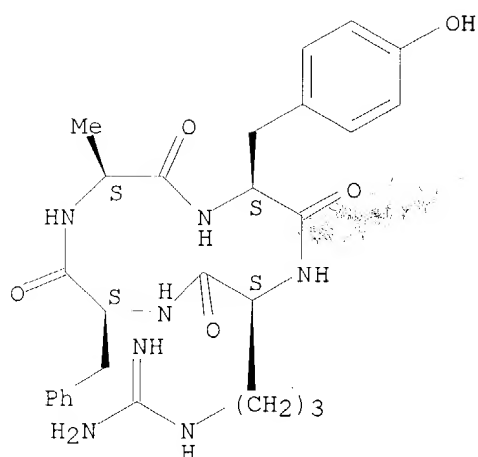
Absolute stereochemistry.



RN 583051-18-7 HCAPLUS

CN Cyclo(L-alanyl-L-tyrosyl-L-arginyl-L-phenylalanyl) (9CI) (CA INDEX NAME)

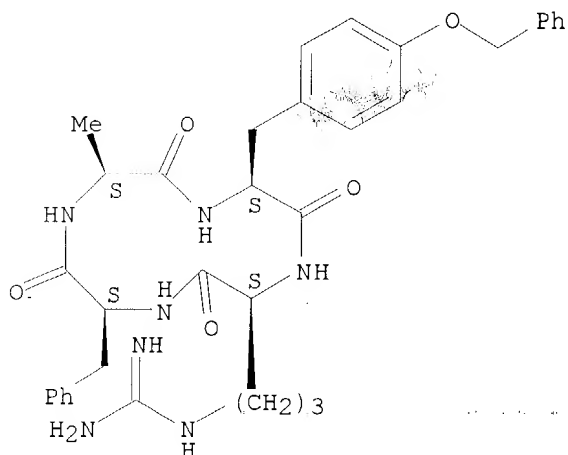
Absolute stereochemistry.



RN 583051-22-3 HCAPLUS

CN Cyclo[L-alanyl-O-(phenylmethyl)-L-tyrosyl-L-arginyl-L-phenylalanyl] (9CI)  
(CA INDEX NAME)

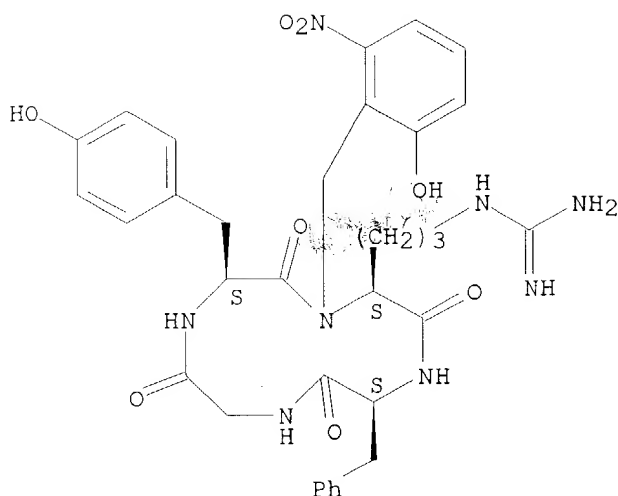
Absolute stereochemistry.



RN 583051-31-4 HCAPLUS

CN Cyclo[N2-[(2-hydroxy-6-nitrophenyl)methyl]-L-arginyl-L-phenylalanylglycyl-L-tyrosyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:227674 HCAPLUS

DOCUMENT NUMBER: 132:265505

TITLE: Solid phase synthesis of small cyclic peptides via on-resin cyclization

INVENTOR(S): Smythe, Mark Leslie; Meutermans, Wim Denise Frans

PATENT ASSIGNEE(S): The University of Queensland, Australia

SOURCE: PCT Int. Appl., 84 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE       |
|---|------|----------|-----------------|------------|
| WO 2000018789   | A1   | 20000406 | WO 1999-AU812   | 19990924   |
| W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM |      |          |                 |            |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  |      |          |                 |            |
| CA 2345067  | AA   | 20000406 | CA 1999-2345067 | 19990924   |
| AU 9963196  | A1   | 20000417 | AU 1999-63196   | 19990924   |
| AU 768649   | B2   | 20031218 |                 |            |
| EP 1115739  | A1   | 20010718 | EP 1999-950390  | 19990924   |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO   |      |          |                 |            |
| JP 2002525376   | T2   | 20020813 | JP 2000-572247  | 19990924   |
| PRIORITY APPLN. INFO.:  |      |          | AU 1998-6165    | A 19980925 |
|   |      |          | WO 1999-AU812   | W 19990924 |

OTHER SOURCE(S): CASREACT 132:265505; MARPAT 132:265505

AB This invention relates to novel auxiliaries for the formation of amide bonds, and to the use of these auxiliaries in a variety of synthetic applications, such as the synthesis of peptides and peptidomimetic compds., and in particular for the synthesis of "small cyclic peptides", so-called "difficult" peptide sequences, and large peptides with a native peptide backbone. The auxiliaries of the invention are also useful in the synthesis of peptides or of C-terminal modified peptides, and in on-resin cyclization of organic mols., ligating chemical, backbone substitution and as backbone linkers. In a particularly preferred embodiment, the invention provides auxiliaries which can be removed by photolysis. Methods of synthesis of a linear or cyclic peptide, a C-terminal modified peptide, or of on-resin cyclization of a peptide mol., comprising the step of linking an amine nitrogen atom to an auxiliary compound of the invention, specific auxiliary compds., which may optionally be linked to a solid support, and kits for synthesis are disclosed and claimed. Thus, cyclo-[Ala-Phe-Leu-Pro-Ala] was prepared via on-resin cyclization reaction.

IT 189031-42-3P 263144-21-4P 263144-23-6P

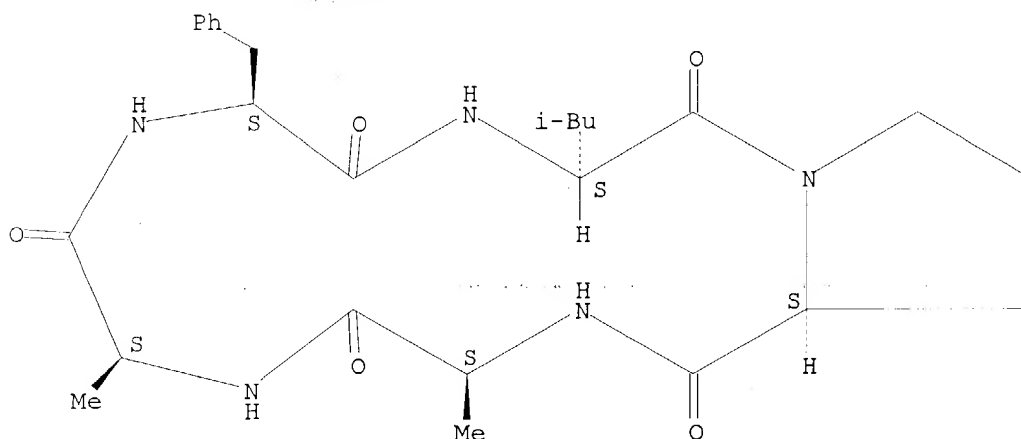
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(solid phase synthesis of small cyclic peptides via on-resin cyclization)

RN 189031-42-3 HCAPLUS

CN Cyclo(L-alanyl-L-alanyl-L-phenylalanyl-L-leucyl-L-prolyl) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

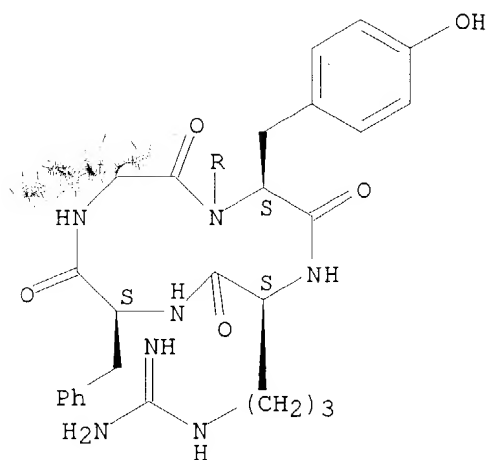


RN 263144-21-4 HCAPLUS

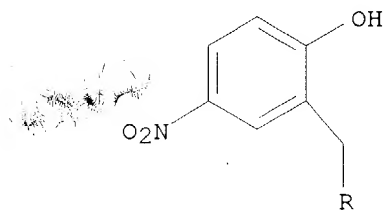
CN Cyclo[L-arginyl-L-phenylalanylglycyl-N-[(2-hydroxy-5-nitrophenyl)methyl]-L-tyrosyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



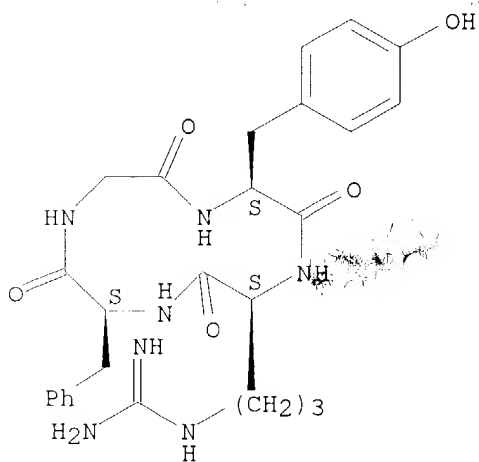
PAGE 2-A



RN 263144-23-6 HCAPLUS

CN Cyclo(L-arginyl-L-phenylalanylglycyl-L-tyrosyl) (9CI) (CA INDEX NAME)

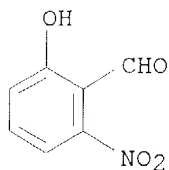
Absolute stereochemistry.



IT 16855-08-6

RN 16855-08-6 HCAPLUS

CN Benzaldehyde, 2-hydroxy-6-nitro- (9CI) (CA INDEX NAME)

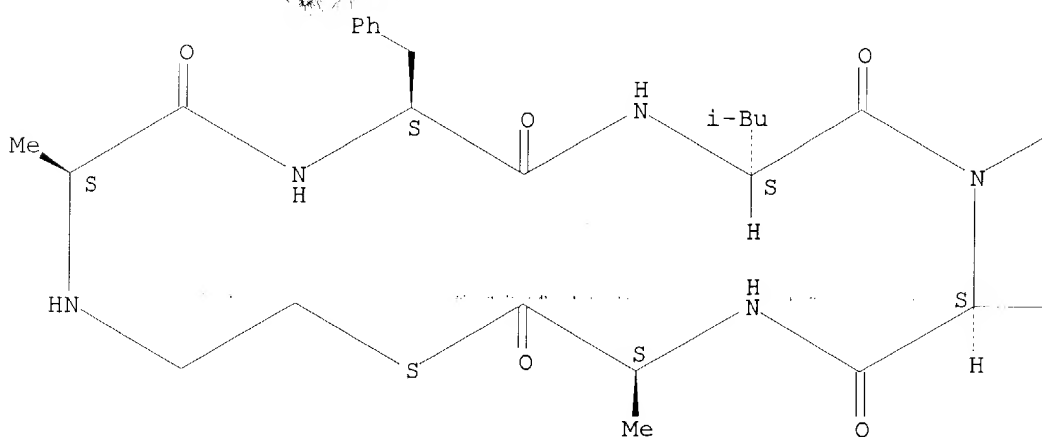


RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(solid phase synthesis of small cyclic peptides via on-resin cyclization)

RN 252667-12-2 HCAPLUS

CN L-Alanine, N-(2-mercaptoethyl)-L-alanyl-L-phenylalanyl-L-leucyl-L-prolyl-,  
(5→1)-thiolactone (9CI) (CA INDEX NAME)

Absolute stereochemistry.



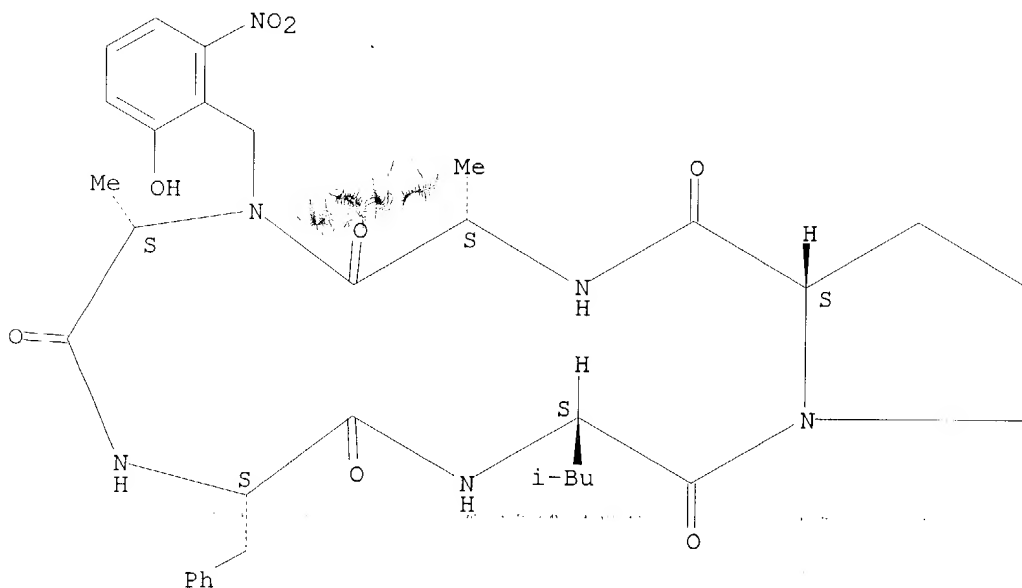
PAGE 1-A

PAGE 1-B



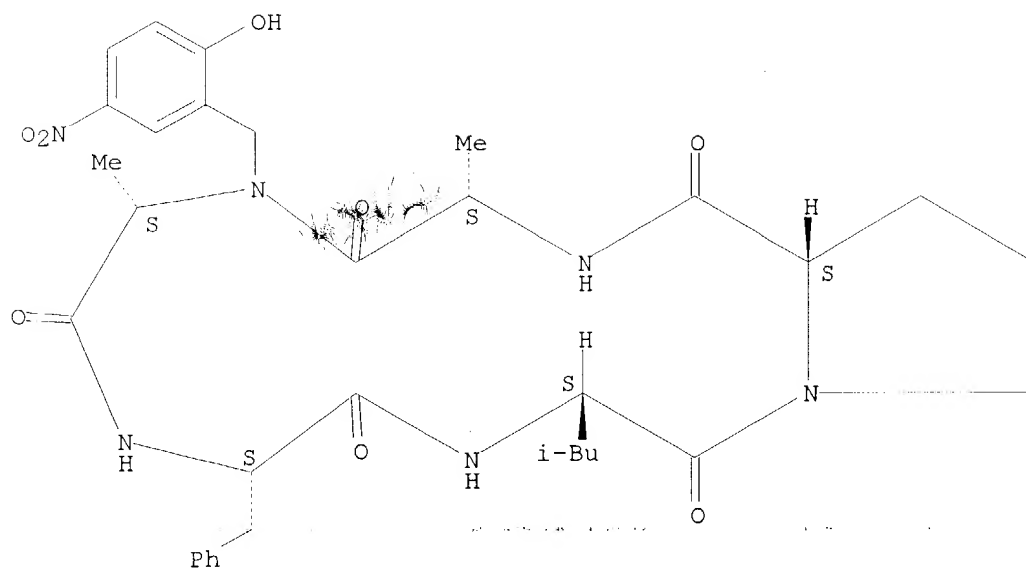
RN 252667-14-4 HCAPLUS  
 CN Cyclo[L-alanyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-alanyl-L-phenylalanyl-L-leucyl-L-prolyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 252667-19-9 HCAPLUS  
 CN Cyclo[L-alanyl-N-[(2-hydroxy-5-nitrophenyl)methyl]-L-alanyl-L-phenylalanyl-L-leucyl-L-prolyl] (9CI) (CA INDEX NAME)

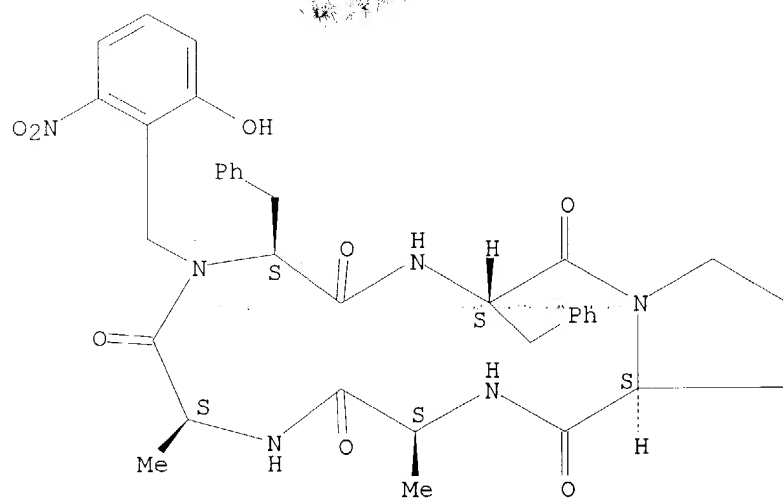
Absolute stereochemistry.



RN 263144-18-9 HCAPLUS

CN Cyclo[L-alanyl-L-alanyl-N-[(2-hydroxy-6-nitrophenyl)methyl]-L-phenylalanyl-L-phenylalanyl-L-prolyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:287131 HCAPLUS

DOCUMENT NUMBER: 131:44797

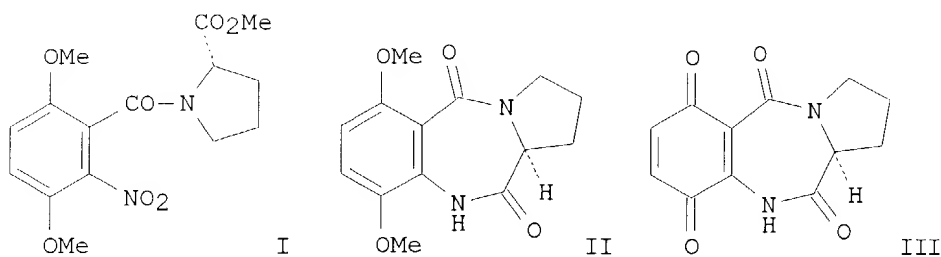
TITLE: Synthesis of a pyrrolo[1,4]benzodiazepinequinone

AUTHOR(S): Tapia, Ricardo A.; Centella, Cesar R.; Valderrama, Jaime A.

CORPORATE SOURCE: Facultad de Quimica, Pontificia Universidad Catolica



SOURCE: de Chile, Santiago, Chile  
Synthetic Communications (1999), 29(12), 2163-2168  
CODEN: SYNCAV; ISSN: 0039-7911  
PUBLISHER: Marcel Dekker, Inc.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Condensation of 3,6-dimethoxy-2-nitrobenzoyl chloride with L-proline Me ester afforded amide I, which underwent reductive cyclization with iron(II) sulfate and ammonium hydroxide to yield pyrrolobenzodiazepine II. Oxidation of II with  $(\text{NH}_4)_2\text{Ce}(\text{NO}_3)_6$  led to the new heterocyclic quinone III in 53% overall yield.

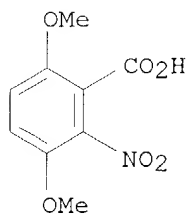
IT 50472-09-8P 50703-23-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn of pyrrolobenzodiazepinequinone via condensation of dimethoxynitrobenzoyl chloride with L-proline Me ester, reductive cyclization, and oxidation)

RN 50472-09-8 HCAPLUS

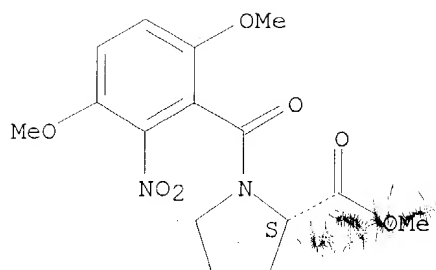
CN Benzoic acid, 3,6-dimethoxy-2-nitro- (6CI, 9CI) (CA INDEX NAME)



RN 50703-23-6 HCAPLUS

CN L-Proline, 1-(3,6-dimethoxy-2-nitrobenzoyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



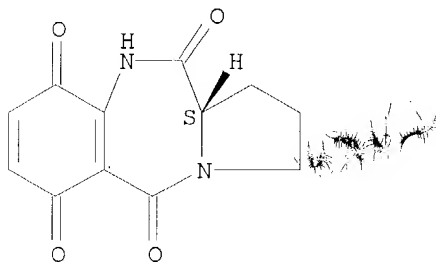
IT 227290-55-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn of pyrrolobenzodiazepinequinone via condensation of  
 dimethoxynitrobenzoyl chloride with L-proline Me ester, reductive  
 cyclization, and oxidation)

RN 227290-55-3 HCAPLUS

CN 1H-Pyrrolo[2,1-c][1,4]benzodiazepine-5,6,9,11(10H,11aH)-tetrone,  
 2,3-dihydro-, (11aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



## REFERENCE COUNT:

19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:134108 HCAPLUS

DOCUMENT NUMBER: 120:134108

TITLE: Intramolecular cycloaddition reactions of dienyl  
 nitroso compounds: application to the synthesis of  
 mitomycin K

AUTHOR(S): Benbow, John W.; McClure, Kim F.; Danishefsky, Samuel  
 J.

CORPORATE SOURCE: Dep. Chem., Yale Univ., New Haven, CT, 06511, USA

SOURCE: Journal of the American Chemical Society (1993),  
 115(26), 12305-14

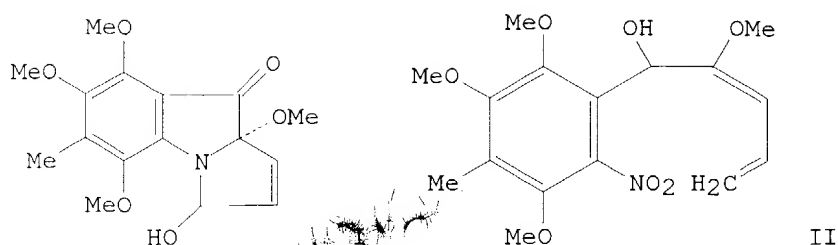
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 120:134108

GI



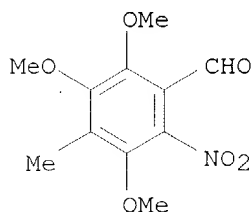
AB The total synthesis of mitomycin K has been achieved. The key reaction produced pyrrolo[1,2-a]indole I from dienyl nitrobenzenemethanol II by a process involving two internal photochem. redox transformations and a [4 + 2] cycloaddn.

IT 113727-24-5 141902-69-4

RL: RCT (Reactant); RACT (Reactant or reagent)  
(intermediate, preparation of mitomycin K)

RN 113727-24-5 HCAPLUS

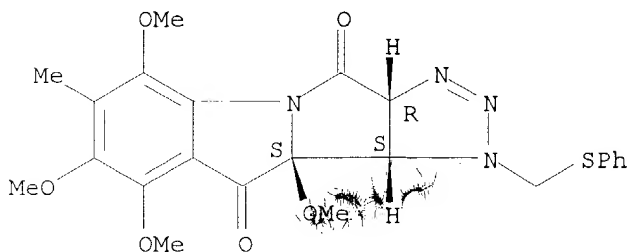
CN Benzaldehyde, 2,3,5-trimethoxy-4-methyl-6-nitro- (9CI) (CA INDEX NAME)



RN 141902-69-4 HCAPLUS

CN 1,2,3-Triazolo[4',5':3,4]pyrrolo[1,2-a]indole-4,10-dione,  
1,3a,10a,10b-tetrahydro-6,8,9,10a-tetramethoxy-7-methyl-1-  
[(phenylthio)methyl]-, (3aα,10aα,10bα)- (9CI) (CA INDEX  
NAME)

Relative stereochemistry.

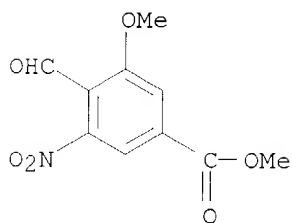


IT 136763-83-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and alkylation of)

RN 136763-83-2 HCAPLUS

CN Benzoic acid, 4-formyl-3-methoxy-5-nitro-, methyl ester (9CI) (CA INDEX NAME)



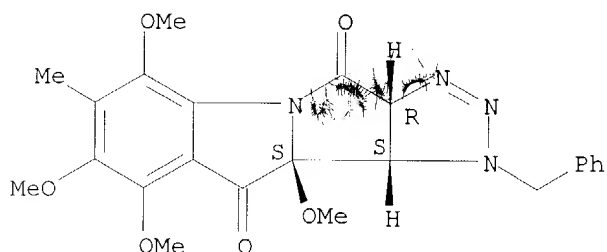
IT 152901-51-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and photolysis of)

RN 152901-51-4 HCAPLUS

CN 1,2,3-Triazolo[4',5':3,4]pyrrolo[1,2-a]indole-4,10-dione, 1,3a,10a,10b-tetrahydro-6,8,9,10b-tetramethoxy-7-methyl-1-(phenylmethyl)-, (3aα,10aα,10bα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



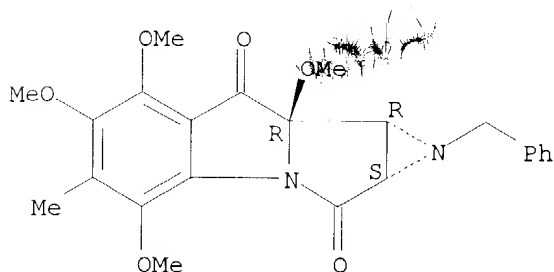
IT 152901-52-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reduction of)

RN 152901-52-5 HCAPLUS

CN Azirino[2',3':3,4]pyrrolo[1,2-a]indole-2,8-dione, 1,1a,8a,8b-tetrahydro-4,6,7,8a-tetramethoxy-5-methyl-1-(phenylmethyl)-, (1aα,8aα,8bα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



W

W

W